CHALMERS
UNIVERSITY OF TECHNOLOGY

Industrial Biotechnology

MULTI-SCALE UNCERTAINTY ANALYSIS

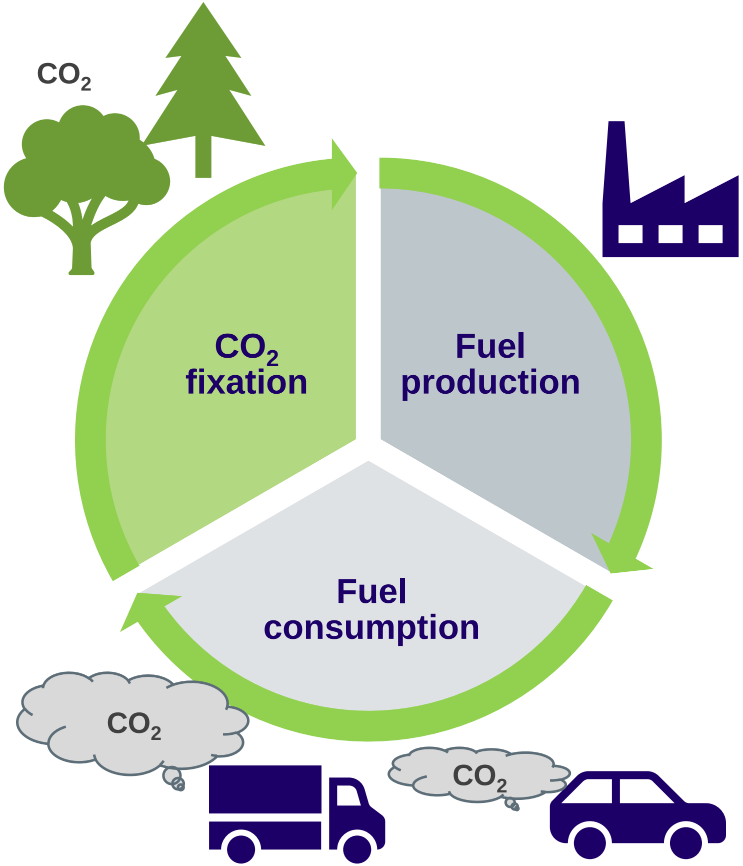
A tool to systematically consider variability in lignocellulosic bioethanol processes

Bioethanol in a circular economy

Usage of fossil fuels steadily increasing

ca. 50% is used for transportation

Bioethanol sustainable alternative to fossil fuels



Variability in the bioethanol process

Raw materials

- Location
- Harvest time
- Composition of biomass
- Storage

Measurement and control

- High turbidity
- Local viscosity differences
- Solid compounds in liquid mixture
- Complex chemical reaction system

Effect of variability on process

Raw material variability

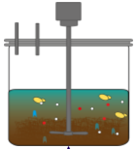
Yields
Productivities

Economy

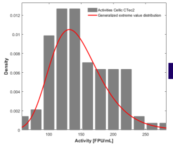
Integrate variability in process development at different scales!

Multi-scale uncertainty analysis – results & objectives

Process definition



Variability/ uncertainty definition



Models at different system scales

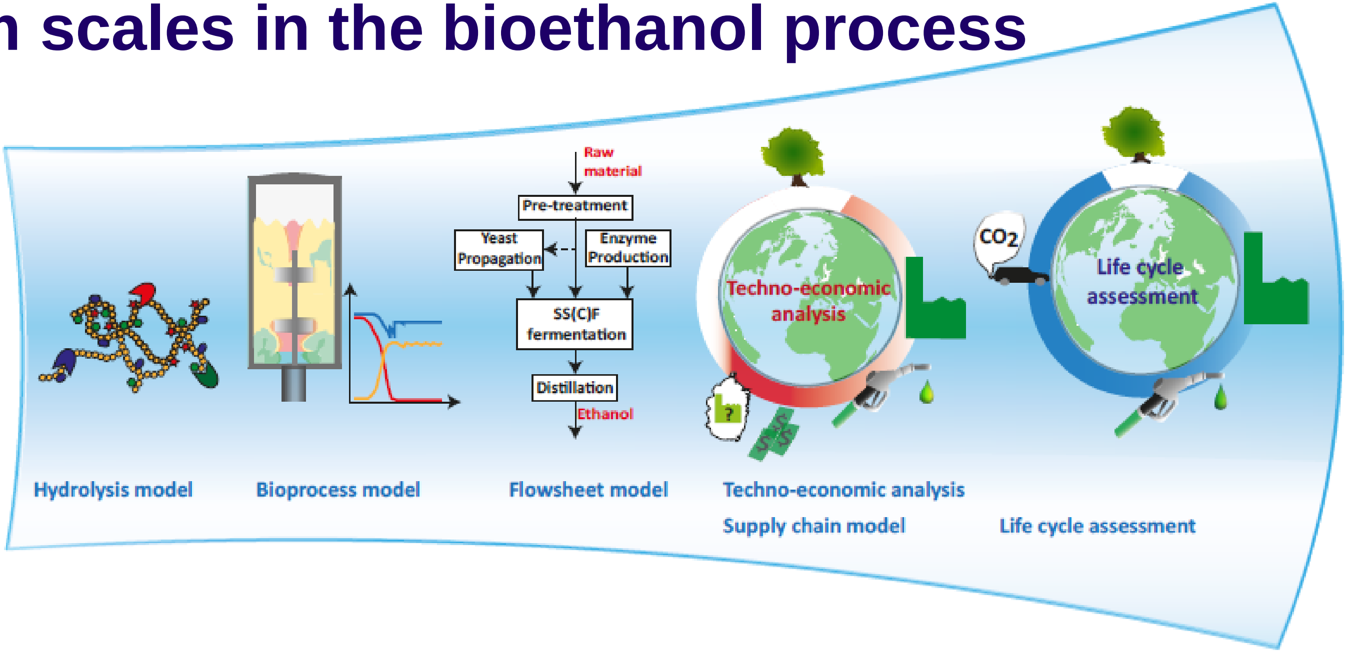
Quantify effect on process outcomes:

- process yield
- process time (productivity)
- process synthesis and design
- process economics
- environmental impact

Consequences:

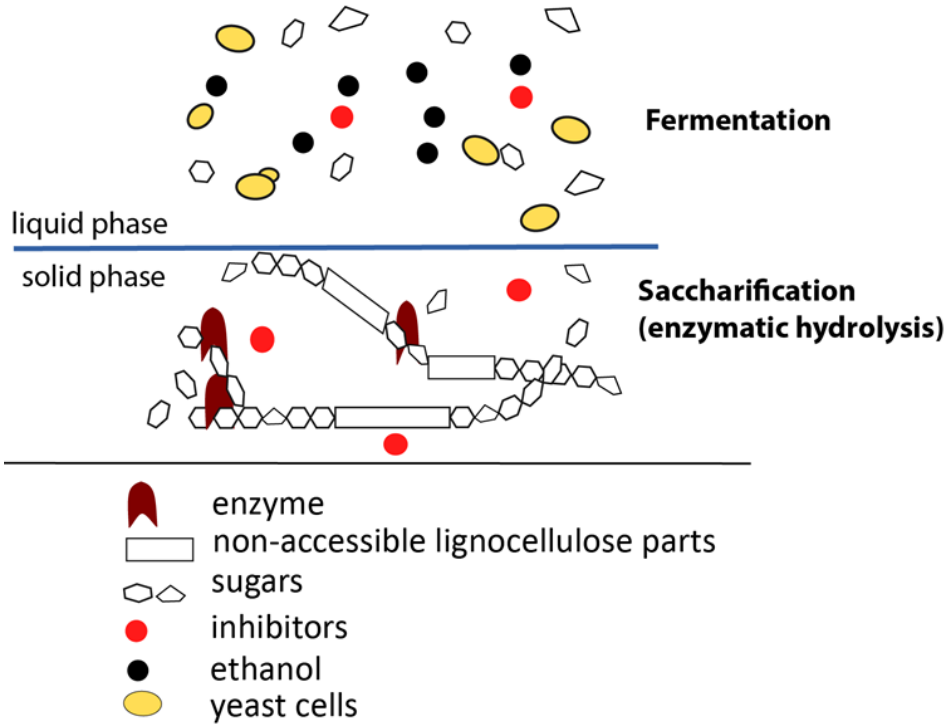
- Improve models (sensitivity analysis)
- Suggest feasible supply chain/ process configurations
- Suggest new experimental procedures

System scales in the bioethanol process



Macro-molecular scale	Bioprocess scale	Factory scale	Global scale	Global scale
describe enzyme action	describe bioprocess	describe process integration	describe cost and profits	describe environmental impact
maximize hydrolysis yield develop enzyme cocktail	develop bioprocess perform optimal experimental designs perform optimal control	develop process synthesis and design	develop supply chain select economically best process alternative(s)	develop process based on environmental impact

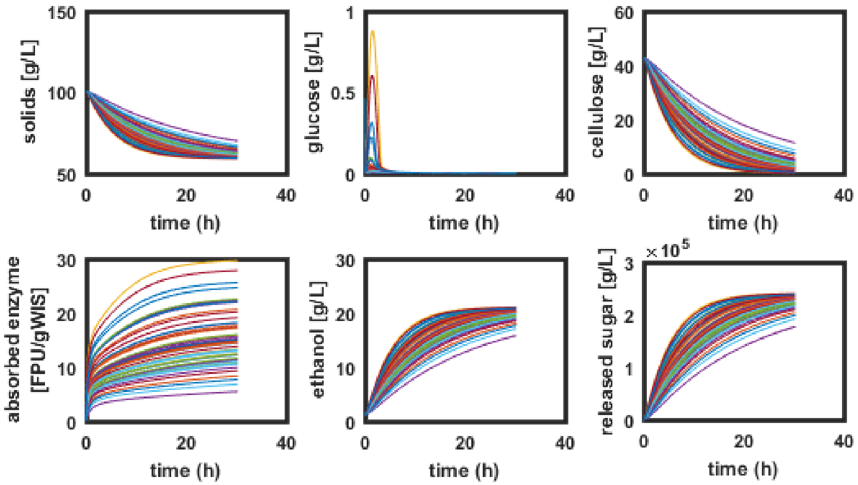
The bioprocess



The bioprocess/ hydrolysis model

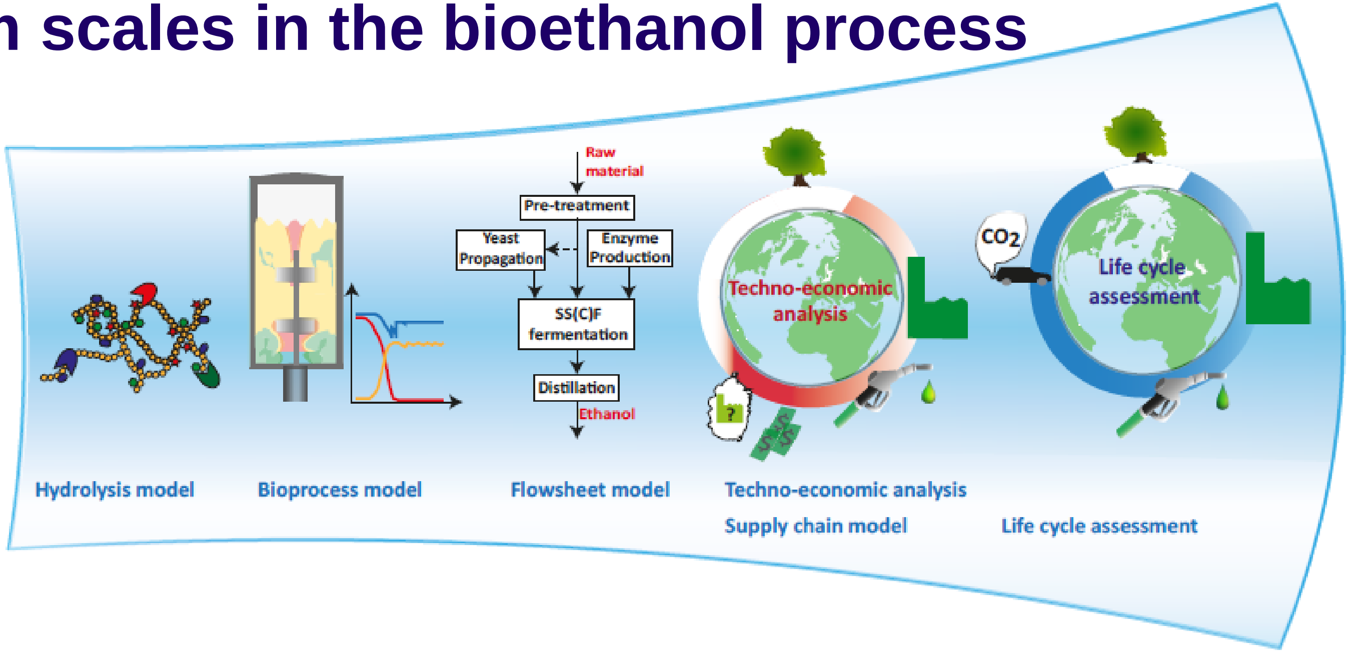
- Macro-kinetic model consisting of
  - 8 differential equations
  - 4 explicit algebraic equations

- Numerical solution in MATLAB using ode15s solver for stiff problems



Simulation results for selected state variables for a batch process at demo plant ($10m^3$) scale

System scales in the bioethanol process



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Flowsheet model and techno-economic analysis

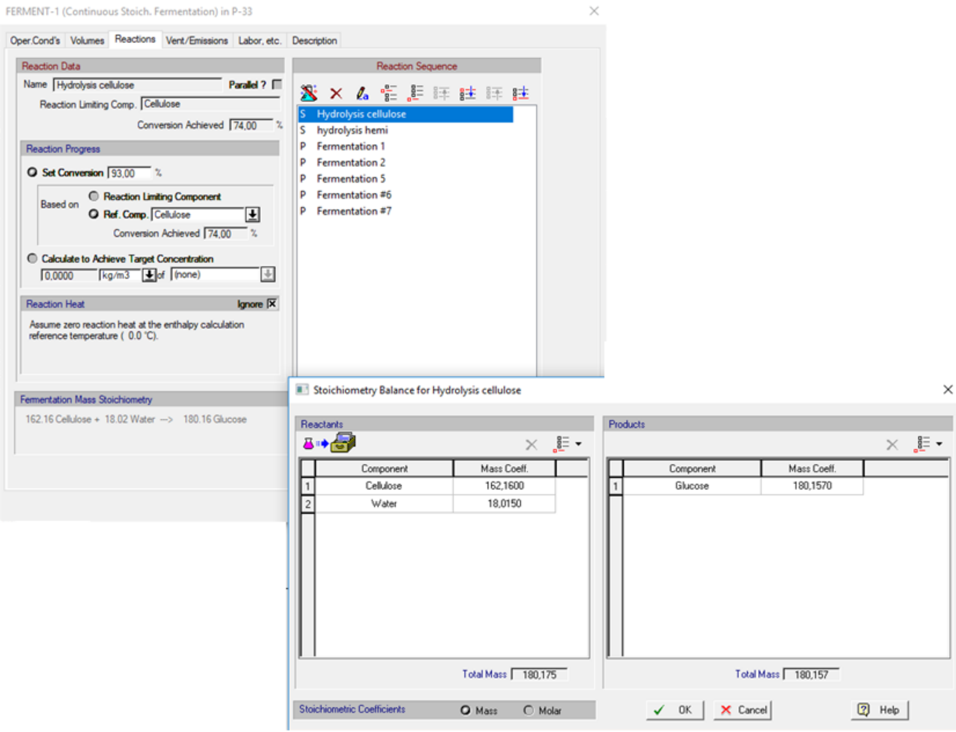
SuperPro Designer

Bioprocess model

OLE server

Process yields

VBA



Flowsheet model and techno-economic analysis

SuperPro Designer

Bioprocess model

OLE server

Process yields

VBA

Yield definitions, mass balances

Experiments

Analyses

External sources

- Process design
- Reactions
- Scheduling
- Utility systems
- Up/downstream units

Bioreactor chain modelling

Flowsheet model and techno-economic analysis

Bioprocess model

OLE server

Process yields

Experiments

Analyses

External sources

- Process design
- Reactions
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- Utility systems
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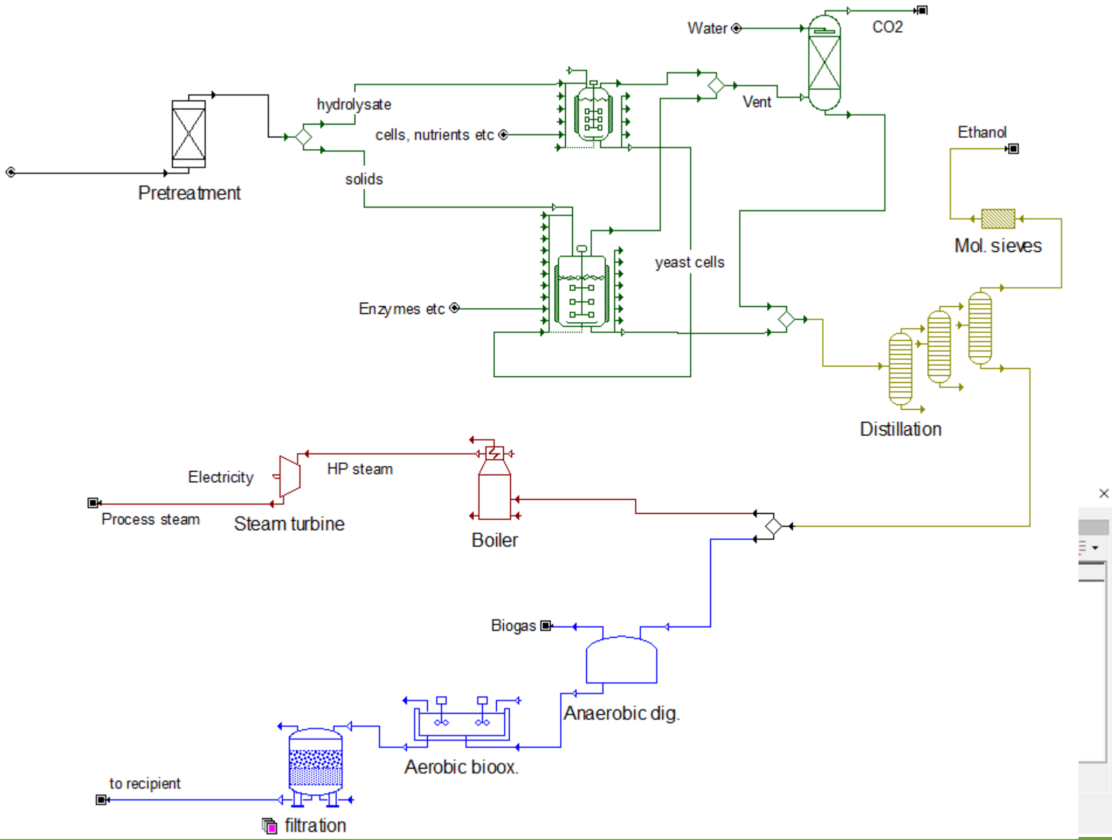
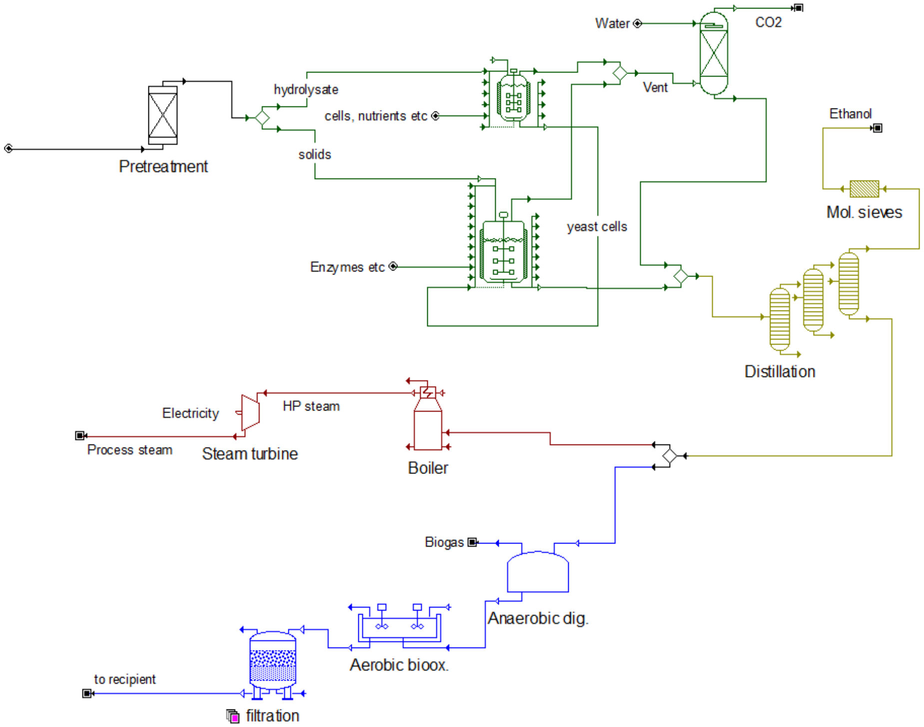
Pinch analysis



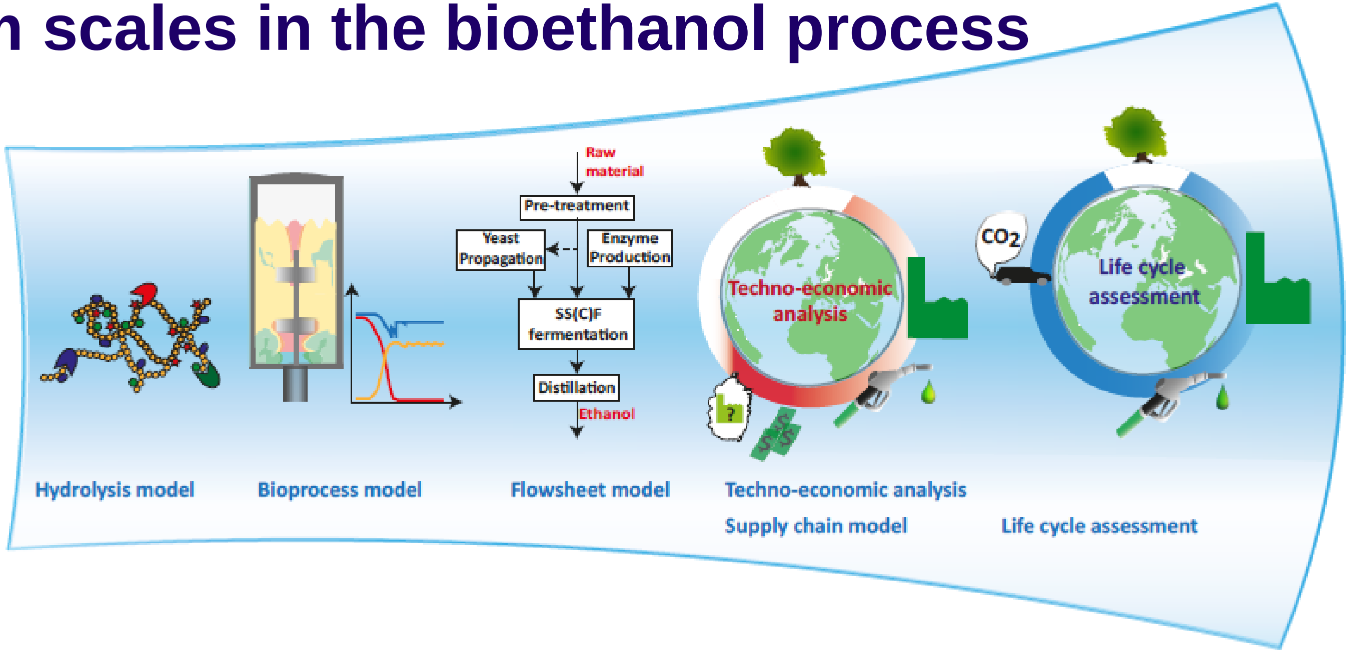
Flowsheet model– the outputs



mass/energy balances to:

- **Techno-Economic Estimates**
- **Supply chain analysis**
- **Life cycle analysis**

System scales in the bioethanol process



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Life cycle assessment

- **Calculates the potential environmental impact of ethanol production**

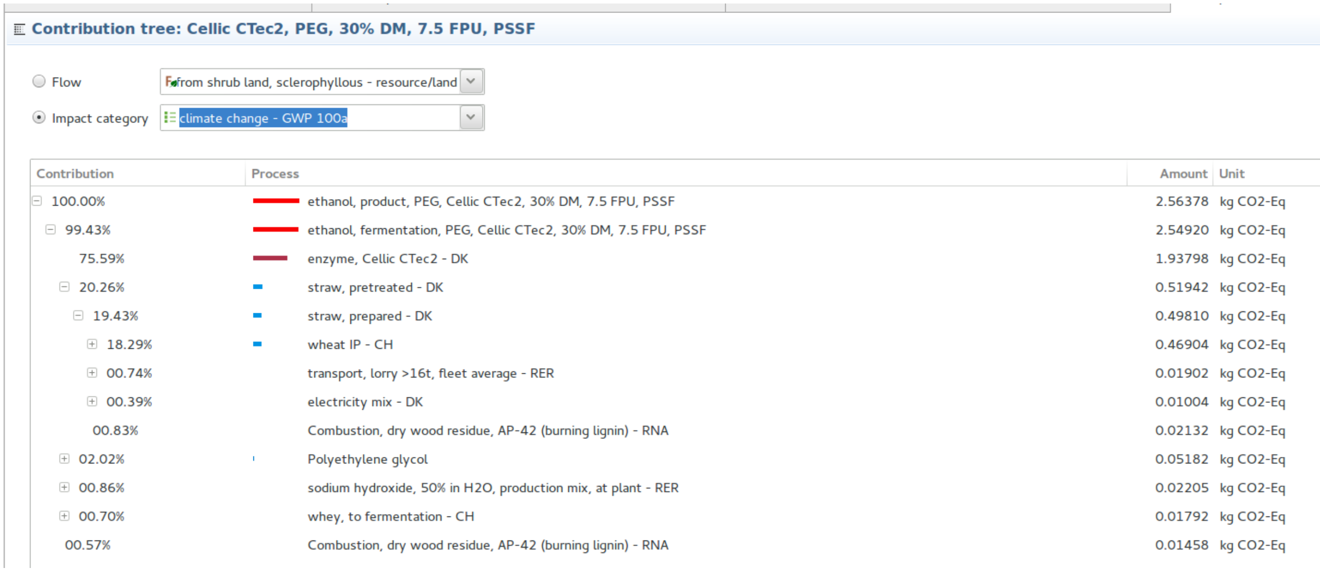
- **Inputs:**

  Database

  Bioreactor model

  Flowsheet model

- **Software: openLCA**



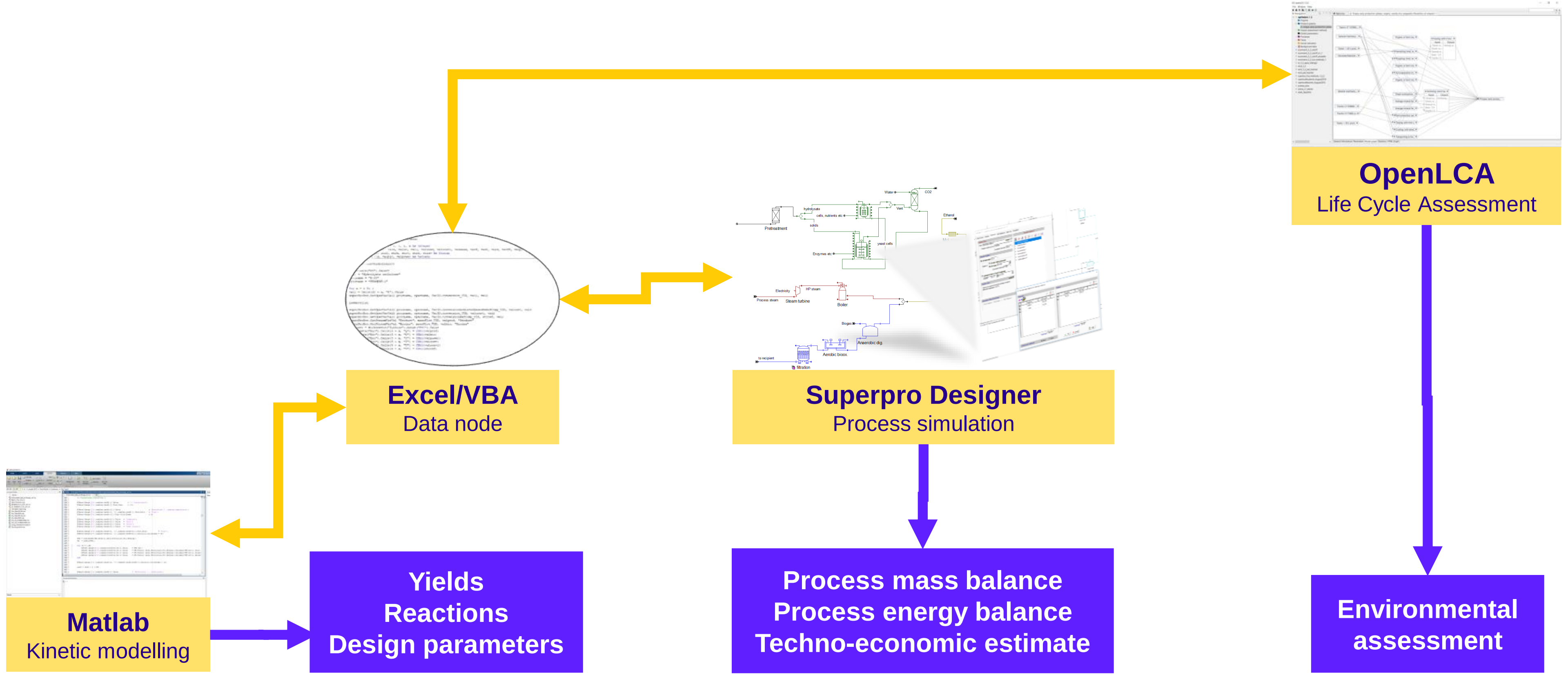
Contribution tree: Cellic CTec2, PEG, 30% DM, 7.5 FPU, PSSF

Flow: From shrub land, sclerophyllous - resource/land

Impact category: climate change - GWP 100a

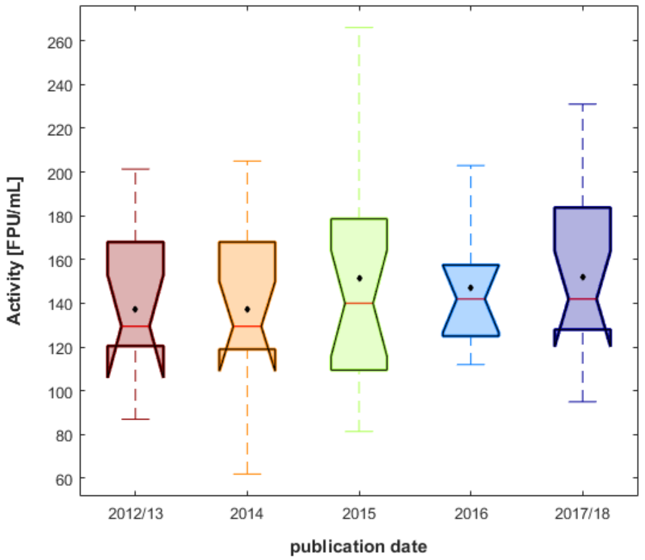
Contribution	Process	Amount	Unit
100.00%	ethanol, product, PEG, Cellic CTec2, 30% DM, 7.5 FPU, PSSF	2.56378	kg CO2-Eq
99.43%	ethanol, fermentation, PEG, Cellic CTec2, 30% DM, 7.5 FPU, PSSF	2.54920	kg CO2-Eq
75.59%	enzyme, Cellic CTec2 - DK	1.93798	kg CO2-Eq
20.26%	straw, pretreated - DK	0.51942	kg CO2-Eq
19.43%	straw, prepared - DK	0.49810	kg CO2-Eq
18.29%	wheat IP - CH	0.46904	kg CO2-Eq
00.74%	transport, lorry >16t, fleet average - RER	0.01902	kg CO2-Eq
00.39%	electricity mix - DK	0.01004	kg CO2-Eq
00.83%	Combustion, dry wood residue, AP-42 (burning lignin) - RNA	0.02132	kg CO2-Eq
02.02%	Polyethylene glycol	0.05182	kg CO2-Eq
00.86%	sodium hydroxide, 50% in H2O, production mix, at plant - RER	0.02205	kg CO2-Eq
00.70%	whey, to fermentation - CH	0.01792	kg CO2-Eq
00.57%	Combustion, dry wood residue, AP-42 (burning lignin) - RNA	0.01458	kg CO2-Eq

Data flow between scales

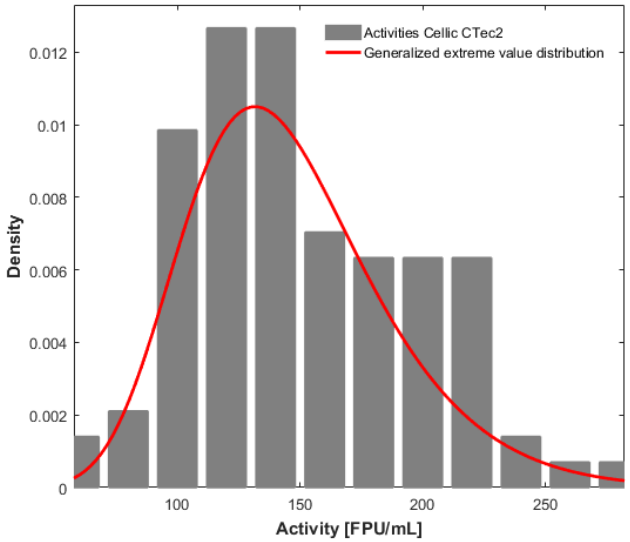


Variability in enzymatic activities – a case study

Step 1: Data collection



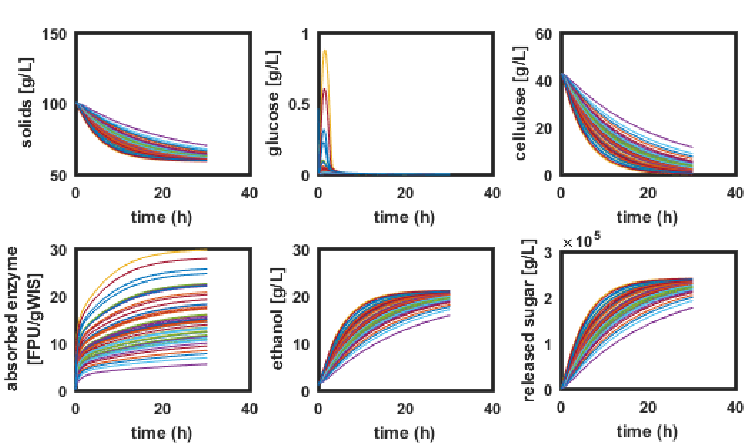
Step 2: Distribution fit



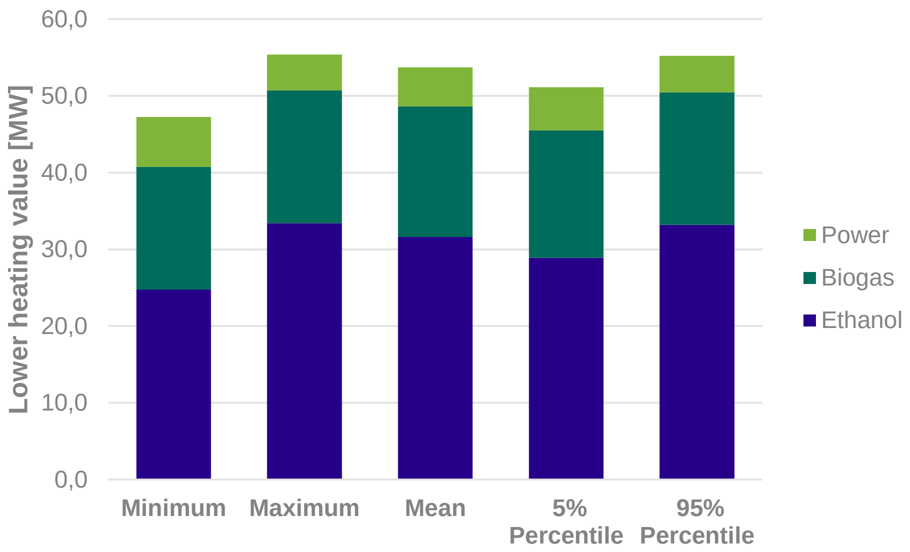
- Generalized extreme value distribution

Variability in enzymatic activities – a case study

Step 3: Propagation in bioprocess model



Step 4: Techno-economic assessment



The multi-scale concept:

- includes variability assessment in early process development
- allows to determine stable process configurations
- allows for multi-objective optimization
- shall allow to determine optimal experimental conditions to perform model validation experiments
- Ongoing: Include life cycle assessment in calculations

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Funded by: Swedish Energy Agency

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